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Monte Carlo simulations of the CP^3 model and U(1) gauge theory in the presence of a θ term

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A θ term, which couples to topological charge, is added to the two-dimensional lattice CP^3 model and $U(1)$ gauge theory. Monte Carlo simulations are performed and compared to strong-coupling character expansions. In certain instances, a flattening behavior occurs in the free-energy at sufficiently large θ, but the effect is an artifact of the simulation methods.

Following the discovery of instanton solutions in four dimensional Yang-Mills theories [1], the importance of adding a θ term $S_\theta = g^2\theta\int d^4x F^a_{\mu\nu}\tilde{F}^{\mu\nu}_a(x)/(32\pi^2)$ to the action was realized [2,3]. Since S_θ breaks parity, time-reversal invariance and CP symmetry when $\theta \neq 0$ or $\theta \neq \pi$, the strong interactions explicitly violate these symmetries for $0 < \theta < \pi$. The physically effective θ angle is bounded experimentally by $\theta_{eff} \lesssim 10^{-9}$ [4,5]. The question of how θ_{eff} can naturally be so small constitutes the strong CP problem in QCD.

Due to the complexity of the problem a preliminary study of simpler systems on the lattice is useful. A class of such systems are the two dimensional CP^{N-1} models [6,7], which have many features in common with four dimensional Yang-Mills theory.

Let us start with a general analysis of simulating systems with θ terms. For the lattice $U(1)$ gauge theory and the CP^{N-1} model, the local topological density ν_p is defined via $\nu_p \equiv \log(U_p)/(2\pi)$, where U_p is the product of the $U(1)$ link phases around the plaquette p and where $-\pi < \log(U_p) \leq \pi$. The total topological charge Q is given by $Q = \sum_p \nu_p$. The theta term $S_{\theta\ \mathrm{term}}$ is $i\theta Q$, that is, [8]

$$S_{\theta\ \mathrm{term}} = \frac{i\theta}{2\pi}\sum_p \log(U_p) \quad . \tag{1}$$

Eq. (1) is the lattice analog of the continuum θ-term action $i\frac{\theta}{2\pi}\int d^2x F_{01}$.

Let $f(\theta)$ be the difference between the free energy $\mathcal{F}(\theta)$ of a system with a θ term and the free energy of a system with $\theta = 0$:

$$f(\theta) = \mathcal{F}(\theta) - \mathcal{F}(0) \quad . \tag{2}$$

Typically, $f(\theta)$ is an increasing function of θ for $0 \leq \theta \leq \pi$. For a fixed volume V, let $P(Q)$ be the probability of having a configuration with topological charge Q in the system. The free energy difference $f(\theta)$ is then constructed from $P(Q)$ using

$$\exp(-Vf(\theta)) = \sum_Q P(Q)\exp(i\theta Q) \quad . \tag{3}$$

Normally $P(-Q) = P(Q)$, so that $f(-\theta) = f(\theta)$.

In a Monte Carlo simulation, an approximation $f_{MC}(\theta)$ to $f(\theta)$ is obtained by using a measured $P_{MC}(Q)$ in lieu of $P(Q)$. Hence

$$-Vf_{MC}(\theta)) = \log\left[\exp(-Vf(\theta)) + \delta Z(\theta)\right] \tag{4}$$

where $\delta Z(\theta) = \sum_Q \delta P(Q)\exp(i\theta Q)$.[1] Since $f(\theta)$ is an increasing function of θ, an accurate measurement of $f(\theta)$ for $0 \leq \theta < \theta_B$ is obtained if

$$|\delta Z(\theta)| \ll \exp(-Vf(\theta_B)) \quad . \tag{5}$$

In particular, since $f(0) = 0$ and $|\delta Z(\theta)| \ll 1$, there is always a region near $\theta = 0$ for which $f(\theta)$ can be measured in a Monte Carlo simulation. However, away from $\theta = 0$, Eq. (5) implies that for sufficiently large V, a limiting value of θ_B exists beyond which it is impossible to reliable

[1]The deviation between Monte Carlo measurements and exact results is denoted by δ.

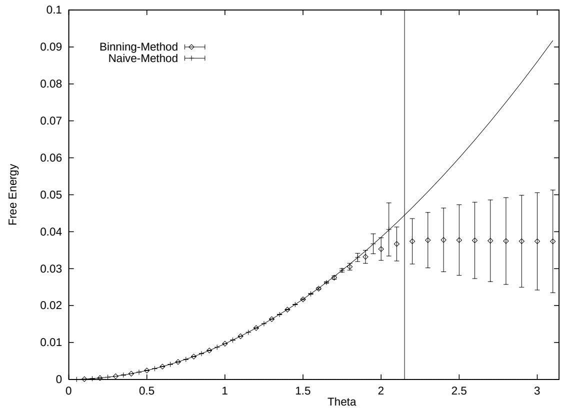

Figure 1. $U(1)$ Free Energy Versus θ at $\beta = 1.0$ for the Naive and Binning Methods.

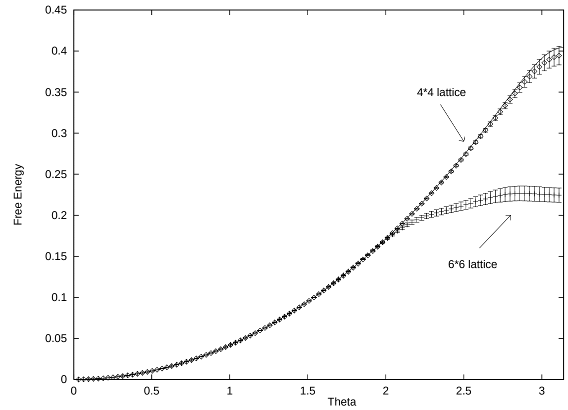

Figure 2. CP^3 Free Energy Versus θ at $\beta = 0.2$ on 4×4 and 6×6 lattices.

compute $f(\theta)$. The value of θ_B depends on the statistical accuracy of the simulation. As V gets larger, θ_B decreases unless enormous numbers of measurements are undertaken to reduce statistical errors. For large V, obtaining enough measurements becomes, in any practical sense, impossible. Clearly, it is more difficult to measure $f(\theta)$ throughout the entire fundamental region of θ, as V gets larger.

It turns out [10] that in most Monte Carlo simulations, there is a tendency for

$$|\delta P(0)| > |\delta P(1)| > |\delta P(2)| > \dots \quad . \tag{6}$$

Now if $|\delta P(0)|$ is much larger than the other $|\delta P(Q)|$ then, from Eq. (5), one deduces an estimate for θ_B

$$f(\theta_B) \approx \frac{1}{V} |\log|\delta P(0)|| \quad . \tag{7}$$

Since Monte Carlo results are reliable for $\theta < \theta_B$,

$$f_{MC}(\theta) \approx f(\theta) \quad \text{for } \theta < \theta_B \quad . \tag{8}$$

If, in addition, $\delta P(0) > 0$, then one finds

$$f_{MC}(\theta) \approx -\frac{1}{V} \log \delta P(0) \quad \text{for } \theta > \theta_B \quad , \tag{9}$$

so that a constant "flat" behavior in $f_{MC}(\theta)$ will be observed, a pure artifact of the simulation. If, on the other hand, $\delta P(0) < 0$, then the measured $f_{MC}(\theta)$ will blow up for $\theta > \theta_B$. In our simulations we have observed both types of behaviours.

From the above discussions we see that as long as finite-size effects are under control, that is $\xi < V^{(1/d)}$,[2] small-volume results for the measurement of $f(\theta)$ are more reliable than large-volume results. If a flattening behavior of the free energy $f(\theta)$ for large θ is observed, one should be cautious that the result is spurious. In particular, one should try to see whether $|\delta P(0)|$ is bigger than the other $|\delta P(Q)|$. Therefore the guideline emerges that if a large-volume simulation shows a flattening effect for $f(\theta)$ for θ sufficiently large, but a smaller-volume simulation does not, one should trust the smaller-volume result.

We note that in the work of [9] a flat behaviour of the free energy was observed and attributed to a phase transition. The results of this work [10] suggest that the flattening is a simulation effect.

The 2-D lattice $U(1)$ gauge theory serves as an ideal testing ground, as computer simulations can be compared to exact analytic results [11]. Figure 1 plots the free energy versus θ for $\beta = 1.0$ on a periodic 16×16 lattice for two different runs. The solid line is the exact analytic result.

[2] Here, ξ is the correlation length and d is the number of dimensions of the system.

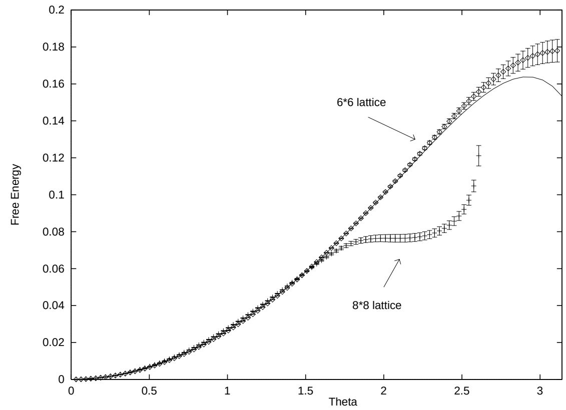

Figure 3. CP^3 Free Energy Versus θ at $\beta = 0.6$ on 6×6 and 8×8 Lattices.

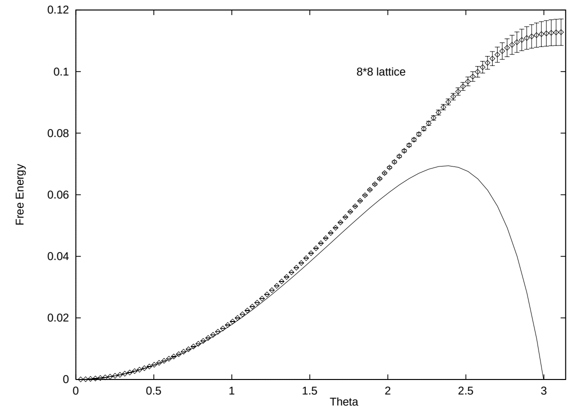

Figure 4. CP^3 Free Energy Versus θ at $\beta = 0.7$ on a 8×8 Lattice.

Both runs have comparable statistics and agree with the analytic results for θ less than 2.1, the value of the “barrier θ” θ_B. Using the known error $\delta P(0)$ in Eq.(7) to estimate θ_B, one finds $\theta_B \approx 2.05$, confirming the above data analysis. The run exhibiting the anomalous flat behaviour in the free energy for $\theta > 2.1$ in fact has a positive $\delta P(0)$, as predicted by Eq. (9).

For the simulations of the lattice CP^3 model[3] we have employed the “auxiliary U(1) field” formulation [13]. Figures 2,3 and 4 show the free energy for $\beta = 0.2, 0.6$ and 0.7 on $4^2, 6^2$ and 8^2 lattices. The solid line represents the tenth-order strong-coupling character expansion of ref. [12]. Figures 2 and 3 show that simulations on smaller lattices are more reliable, as the simulations on the larger lattices exhibit anomalous flattening. Again the estimated θ_B for these simulations was in good agreement with the observed one. In the intermediate coupling regime of $\beta = 0.7$ in figure 4 the Monte Carlo data is most likely to be trusted over the strong-coupling expansion. Curiously for higher values of β the MC simulations were nicely fitted by a cosine [10], which also arises from a topological gas picture [2].

[3]For simulations without a θ term see refs. in [10]

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